CHEMISTRY AND MATERIALS SCIENCE DIRFCTORATE NEWS



Message from the Associate Director

Recently, we conducted an anonymous survey to evaluate the effectiveness of the directorate's communications. Participants were asked to evaluate media and mechanisms by which information was disseminated. Overall, 229 people responded to our survey, providing valuable insights that will surely influence the course of our future efforts.

I want to thank everyone for taking the time to complete the survey. I also want to share with you some of the results and our initial action plan.

Gauging by how participants ranked various communications efforts, we were encouraged by the positive feedback in several areas, including safety, security, and overall scientific visibility. Most gave high grades to communication techniques and effectiveness.

While we will continue the positive aspects of directorate communications, we are identifying areas for improvement and redirecting our internal resources to broaden the benefits in these areas. Our goal is not simply to increase the volume of information but rather to target the needed resources to the right audience.

In addition, we plan to unveil new campaigns to further strengthen our safety culture and promote employee participation. We want to fully embrace our emphasis on simultaneous excellence in operations and science, encouraging our employees to achieve this goal.

The survey results also reflected a common interest for more information on career development and IPPP

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Corner on Science

Studying Alloys Made to Last Millennia

The current design for nuclear waste containers in the repository at Yucca Mountain consists of an inner canister of stainless steel and an outer container of a nickel-chromium-molybdenum alloy, called Alloy 22. The containers are required to maintain integrity without substantial leakage for several thousand years. A team is evaluating the effects that fabrication processes can have on the performance of these materials by determining the aging kinetics, material properties, phase stability, and corrosion resistance under repository conditions. Sharon G.

Torres of the Materials Science and Technology Division is leading this team, which is characterizing the microstructure and providing experimental data on the phase stability of Alloy 22. Post-doc Bassem El-Dasher developed a method using electron backscatter diffraction (EBSD) for identifying and quantifying tetrahedrally close-packed (TCP) phases in Alloy 22, which are known to increase the materials' susceptibility to corrosion and mechanical degradation.

Not only does EBSD allow the identification of the TCP phases (all of



Clockwise from top left: Sharon Torres, Tanya Reshel, Bassem El-Dasher, and Mike McGregor.

different crystal structures), but large areas of the specimens can be characterized as well. EBSD is currently the only method being applied that accumulates sufficient data to provide statistical accuracy. A computer model predicting the microstructural evolution of these phases over thousands of years is verified by comparison to specimens that have been aged at elevated temperatures. **Mike McGregor** and **Tanya Reshel** maintain the facilities in which hundreds of samples have been

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Interview with ... Nina Rosenberg



Nina Rosenberg, recently appointed Division Leader of the Chemical Biology and Nuclear Science Division (CBND), looks forward to doing her utmost to enhance and expand the excellent work being done in the division.

After earning a Ph.D. in geological sciences at the University of California at Santa Barbara in 1991, Nina started her career at Los Alamos National Laboratory (LANL). She became a LANL research fellow at the University of California at Santa Cruz and then moved to LLNL in 1998 as a geoscientist in the Energy and Environment Directorate. She joined the CMS directorate two and one-half years ago.

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CMS Directorate Review

DRC Takes a Close Look at CMS Contributions to Key DNT and NIF Programs



Alex Hamza, John Rogers, University of Illinois, Urbana-Champaign, and **Jeff Kass** (left to right) relax after giving excellent presentations about NIF target material development.

On May 23-25, 2005, the CMS Directorate Review Committee (DRC) evaluated CMS research and program support in three areas: plutonium aging, fabricating targets for the National Ignition Facility, and materials dynamics and ultrafast science. All three areas are of critical importance to stockpile stewardship.



Evan Reed discusses predicting how coherent terahertz photons emerge from shock waves in crystals.

The DRC found that CMS is doing an outstanding job in support of National Nuclear Security Administration and Laboratory programs. DRC Chairman **John Poate** wrote, "the scientific and technology base underlying the three programs is world class and we assign a grade of outstanding for Performance Objective/Measure 5."

CMS People

CMS Staff Win Four R&D 100s

CMS employees figured prominently in three of the four R&D 100 awards that the Laboratory won this year. A CMS staffer was also part of a team from Lawrence Berkeley National Laboratory (LBL) that won an award. Congratulations to all!



The bioaerosol mass spectrometry (BAMS) system, developed in support of homeland security, can sort out a single spore from thousands of other biological and nonbiological particles with no false positives. The team includes (left to right, back row) Paul Steele, Todd Weisgraber, Bruce Woods, Abneesh Srivastava, and **Keith Coffee**; (middle row) Vincent Riot, Jim Birch, **Herbert Tobias**, and **Eric Gard**; (front row) Matthias Frank and **David Fergenson**.



Henry Benner was a member of the LBL team that developed ion mobility analysis to measure the size distribution and count the number of individual particles in

Henry Benner

lipoproteins (fats). This analysis of the size, quantity, and type of lipoprotein particles provides a far better indicator than standard cholesterol testing of whether someone is at risk for heart disease.



Troy Barbee

NanoFoil is a revolutionary product that creates a strong, thermally conductive bond to join metals, ceramics, semiconductors, and polymers. The NanoFoil technology grew out of multilayer, nanolaminate research started by **Troy Barbee**. The technology was developed further and commercialized by a former post-doc of Barbee's.

CMS People Continued from page 2





David Trombino

Dan Archer

David Trombino and former Laboratory employee **Dan Archer** were members of the team that developed the adaptable radiation area monitor (ARAM). ARAM detectors are designed for fast, accurate detection of even small amounts of radiation in a vehicle moving at highway speeds.

Interview with. . .

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Nina studied the flow and transport of fluids in the Earth and their chemical interactions, especially under hydrothermal conditions. Nina's experience in examining contaminant transport at LANL brought her to the LLNL Yucca Mountain Project. There she developed new data on the geothermal and geochemical conditions caused by heat from radioactive waste containers interacting with groundwater. She eventually became Deputy Program Leader in the Nonproliferation, Arms Control, and International Security (NAI) Technology Program Office and CMS Deputy Materials Program Leader for NAI.

When CMS Associate Director Tomás Díaz de la Rubia announced her appointment, he noted, "Dr. Rosenberg brings ... a proven ability to build bridges between people and organizations." As CMS division leader, Nina looks forward to building yet more bridges: creating opportunities for CBND scientists to better connect with programmatic work at the Laboratory.



Spotlight on...Recently Published Work

Complex Inorganic Solids

Patrice Turchi is one of the editors of this Springer Verlag (New York, ISBN 0387248110) book with the subtitle of "Structural, Stability, and Magnetic Properties of Alloys." This book highlights commonalities among different fields of alloy research, ranging from geology to metallurgical engineering. The papers are organized into the categories of microstructural considerations, ordering, kinetics and diffusion, magnetic considerations, and elastic considerations.

Molecular Modeling Techniques in Material Sciences

Amitesh Maiti is one of three authors of this just-published overview of methods of molecular modeling (CRC Press, ISBN 0824724194). Methods include modeling metal oxides, microporous materials, glass, semiconductors and superconductors, and nanomaterials.

Microbial Forensics

Published by Academic Press (ISBN 0120884836), chapter 13, entitled "Non-DNA Methods for Biological Signatures," includes, along with six other Lab contributors, many from CMS: Charlene Schaldach, James DeYoreo, Tony Esposito, David Fergenson, Eric Gard, Christopher Hollars, Thomas Huser, Alexander Malkin, Maurice Pitesky, Chad Talley, Herb Tobias, Patrick Grant, James Ferreira, Kuang-Jen Wu, and Joanne Horn. Their chapter covers the intrinsic molecular properties of

fingerprints, a multidisciplinary approach to biological signatures, details of individual methods, an analysis of spore samples, and a discussion of future directions.

New Hot Paper

In the materials science field for July 2005, the Thomson ISI New Hot Paper selected **Yinmin (Morris) Wang's** paper, which was published in volume 52(6) of *Acta Materialia* and entitled "Three strategies to achieve uniform tensile deformation in a nanostructured metal." His invited comments can be found at www.esi-topics.com/nhp/2005/july-05-YinminMorrisWang. html.

Nanotube Research Recognized in *Materials Today*

An article in the July/August edition of *Materials Today* acknowledged the work of **Aleksandr Noy** and coworkers, along with colleagues at the University of California at Davis. The article noted that this group's paper on nanotube templates has recently been published in the *Journal of the American Chemical Society*. [(Artyukhin et al. *J. Am. Chem. Soc.* **127**(20), 7538 (2005)].

Please send items for the next newsletter (e.g., directorate news, awards) to **Stephanie Shang** (shang2@llnl.gov)

Corner on Science

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aging 24/7 for the past seven years. They also prepare the specimens for EBSD analysis.

The team is studying Alloy 22 welds as well. Welds are inherently inhomogeneous, and any microstructural characterization must be conducted over large (centimeter) length scales. However, TCP phases are small, requiring a submicron resolution for observation. To overcome these conflicting demands, a method was developed that combines conventional scanning

electron microscope imaging with EBSD to map 2-cm^2 sections of a weld at a resolution of $0.5~\mu m$... approximately equivalent to mapping the contiguous United States and being able to see every car on the road!

The team also collaborates on other Yucca Mountain work, including a study with **Christine Orme** and **Jeremy Gray** to rapidly assess the corrosion properties of polycrystalline Alloy 22 in various acidic environments. Another collaborative study with **Frank Wong**

investigates the metallurgy and feasibility of electron-beam welding of Alloy 22.

ASM International recently presented Bassem and four other researchers with the Henry Marion Howe Award. This annual award honors the best paper published in a specific volume of *Metallurgical and Materials Transactions*. 1

¹Saylor, D.; Fridy, J.; El-Dasher, B.; Jung, K.; Rollet, A. Statistically Representative Three-Dimensional Microstructures Based on Orthogonal Observation Sections. *Metall. Mater. Trans. A* **35A**, 1969–1979, July 2004.

Message from the Associate Director

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(Integrated Performance and Pay Program). We recognize the individual needs of our employees, and we are assessing ways to address these issues.

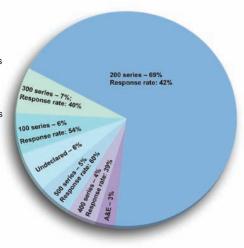
During the upcoming all-hands meeting in November, I will cover in greater detail what we learned from the survey and our action plan. These results will help us establish a benchmark from which to measure our progress.

This survey is only the first step in our renewed commitment to excellence in communications and to doing our best in everything, despite constraints. Your involvement, together with management commitment, will be critical in our effort to improve the communication processes in the directorate.

Tomás

This pie chart shows percent of respondents represented by each job series (200 series = 69%).

"Response rate" shows percent of employees in each series that responded to survey.



Upcoming Events

DATE	EVENT	LOCATION	WEB SITE
Nov. 14-16	LLNL BioSecurity S&T Director's Review Committee	LLNL	N/A
Nov. 28–30	Materials Research Society Fall Meeting	Boston, MA	http://www.mrs.org/meetings/fall2005/program/f05_pgm_h.html>
Mar. 26–30	ACS Spring Meeting	Atlanta, GA	http://acswebcontent.acs.org/home.html

To be added to the CMS Newsletter mailing list, contact Galen Hazelhofer (hazelhofer1@llnl.gov)

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